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(54) Title: CONFORMATIONAL SAMPLING BY SELF-ORGANIZATION

(57) Abstract: A self-organizing method, system, and computer program product for generating molecular conformations that are consistent with a set of distance and/or volume constraints. A stochastic proximity embedding (SPE) algorithm evaluates individual distance and/or volume constraints and adjusts the atomic coordinates to minimize violations of such constraints. The method scales linearly with thenumber of atoms, and produces many more unique conformations at a fraction of the time required by conventional distance geometry algorithms.

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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US03/19905

A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 33/48

US CL : 702/19

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 702/19

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
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C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	FEUSTON et al. Comparison of Knowledge-based and Distance Geometry. Approaches for Generation of Molecular Conformation. J. Chem. Inf. Comput. Sci. 2001, Vol. 41, pages 754-763. Entire document.	1-12
Y	HUANG et al. Distance Geometry Generates Native-like Folds for Small Helical Proteins Using the Consensus Distances of Predicted Protein Structures. Protein Science. 1998, Vol. 7, pages 1998-2003. Entire document.	1-12
A	US 6,269,312 B1 (MAYO et al) 31 July 2001 (31.07.2001) especially columns 5-72.	1-12
A	US 5,241,470 A (LEE et al) 31 August 1993 (31.08.1993), especially columns 4-27.	1-12
A	US 5,553,004 A (GRONBECH-JENSEN et al) 03 September 1996 (03.09.1996), especially columns 6-26.	1-12
A	US 6,150,179 A (WENT) 21 NOVEMBER 2000 (21.11.2000), especially columns 5-61.	1-12



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Continuation of B. FIELDS SEARCHED Item 3:
EAST and STN